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Transport properties of gas mixtures

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Abstract : A method for estimating transport coefficients of binary and multicomponent gas mixtures has been proposed. Deviations of the results predicted are of the same order as the uncertainty in experimental measurements Finally comments on the improved corresponding states principle have been given.

Keywords Transport coefficients, binary and multicomponent gas mixtures

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ntroduction

re has been continued interest in the study and estimation ansport properties of gas mixtures [4,7,9]. General essions have been worked out with the Chapman-Enskog iod [4,13] which related the transport coefficients to the known collision integrals. These expressions give the er-order contributions whose evaluation for a given molecular potential is a cumbersome job. Keeping in of the accuracy of the available transport coefficient computation of higher-order contribution is a must. To ply the job, approximate relations for estimating these ributions to viscosity and thermal conductivity of gas s have also been attempted [10,12]. An alternative oach, based on the first order kinetic theory expressions ugh the use universal functionals [7,8] has been quite factory in reproducing the transport coefficient data in experimental uncertainty.

The purpose of the present work is to propose a method timate viscosity and thermal conductivity of gas mixtures ch takes into account the higher-order contribution in a plified manner. In Section 2 expressions have been given the proposed method of estimation. Results of putation for binary and ternary mixtures (along with entage deviation from accurate experimental data) and comparison with those from the corresponding states principle have been discussed in Section 3. Finally, comments on the inconsistent procedure of the improved corresponding states principle have been given.

2. Expressions

Viscosity of a gas mixture is given by,

$$\eta_{\text{mix}} = [\eta_{\text{mix}}]_1 f_{\eta_{\text{mix}}} \tag{1}$$

where $[\eta_{\text{mix}}]_1$ is the first-order viscosity of the gas mixture obtained from expression ([4], eq. 11–34 of Ref. [7]). The first-order values $[\eta_i]_1$ are obtained through the use of universal functional such as $\Omega^{(2,2)}$, $\Omega^{(1,1)}$, ... *etc.* The higher-order contribution to the mixture viscosity is given by

$$f_{\eta_{\text{mix}}} = X_1^2 f_{\eta_1} + X_2^2 f_{\eta_2} + 2X_1X_2 f_{\eta_{12}} \tag{2a}$$

for a binary mixture [3]

$$f_{\eta_{\text{mix}}} = \sum_{i=1}^{N} X_i^2 f_{\eta_i} + \sum_{i,j=1}^{N} X_i X_j f_{\eta_{ij}} \tag{2b}$$

for a multicomponent mixture [10]

where $f_{\eta_{ij}} = 1 + 3/196 * (8E_{ij} - 7)^2$ (3)

$$E_{ij}^* = \Omega_{ij}^{(2,3)^*}(T_{ij}^*) / \Omega_{ij}^{(2,2)^*}(T_{ij}^*)$$

and $f = f$

Similarly thermal conductivity of a gas mixture

$$\lambda_{mix} = [\lambda_{mix}]_1 f_{\lambda_{mix}} \tag{4}$$

where $[\eta_{mix}]_1$ is the first-order thermal conductivity obtained from the expression ([4], eq. 11.40 of Ref. [7] with $f_{ij} = 1$). The higher order contribution to the mixture thermal conductivity is given by

$$f_{\lambda_{mix}} = X_1 f_{\lambda_1} + X_2 f_{\lambda_2} + CX_1X_2(f_{\lambda_{12}} - 1) \tag{5a}$$

for a binary mixture [11] and

$$f_{\lambda_{mix}} = \sum_{i=1}^{N} X_i f_{\lambda_i} + \sum_{\substack{i,j=1 \\ i \neq j}}^{N} C_{ij} X_i X_j ({}^{O}f_{\lambda ij} - 1) \tag{5b}$$

for N-component mixture [12]

where $f_{\eta_{ij}} = 1 + 1/42^{*}(8E_{ij}^{*} - 7)^2$ (6)

and $f = f$

Apparenty inconsistent procedure of the improved Corresponding States Principle makes use of the first order kinetic thoery expressions wherein only the first order values the transport coefficients are replaced by their higher order values with the help of the functionals $\Omega^{(2,2)}$, $\Omega^{(1,1)}$, ... *etc.* [8]. This procedure could be made cosistent through the use of approximate relations for the higher-order contribution (equations (2) and (5)).

3. Computation and results

Using expressions (1) and (2) viscosity of binary He–Xe and ternary He–Ne–Xe mixture has been computed and the results have been placed in Table 1 along with those obtained from the corresponding states principle [7]. Experimental values have been taken from Kestin *et al* [5,6]. Similar computations for thermal conductivity have been presented in Table 2. Here experimental values have been taken from Clifford *et al* [2]. Viscosity and thermal conductivity data are accurate to within 0.1 and 0.2 percent respectively. It has been observed that especially for mixture with large mass-ratios such as He–Ar (M_2/M_1 = 9.98) the results for thermal conductivity with the proposed method appear to be in good agreement rather than those with the Corresponding States Principle. Further improvement in the predicted results is expected with the modification of eqn. (6) (such that it matches the third order contribution to thermal conductivity). Moreover labour involved in the above mentioned procedure is almost the same universal functionals are to be used.

Table 1. Experimental values η_{exp} and Percentage Deviatic PD (= $(\eta_{exp} - \eta_{mix})/\eta_{exp} \times 100$) for viscosity of He–Xe and He–Ne mixtures for the various compositions and temperatures

Mixture	Tempe-rature T(K)	Compo-sition	η_{exp} (μ P)	PD Eqns. (1) and (2)	CSP
		I	241.78	0.23	0
	298	II	254.43	0.02	0
		III	255.03	−0 45	−0
He–Xe		I	552.13	0 01	0
	778	II	558.48	0 04	0
		III	513.54	−0 16	0
	298	IV	275.05	−0 38	0
	373	IV	334.22	−0.08	0
He–Ne–Kr	483	IV	399.21	−0 07	0
	573	IV	448.79	−0 02	0
	673	IV	498 95	−0 38	0

Composition	X_1	X_2	X_3
I	0.2677	0 7323	
II	0.5316	0 4684	-
III	0 8687	0 1313	-
IV	0.5435	0 3282	0 1283

CSP ⇒ Corresponding States Principle [eqns (11–34) page 267 Millat *et al* (1996)]

Table 2. Experimental values λ_{exp} and Percentage Deviat PD (= $(\lambda_{exp} - \lambda_{mix})/\lambda_{exp} \times 100$) for thermal conductivity of Ne–Ar a He–Ar mixtures for the various compositions at 300 5 K

Mix-ture	Mass-ratio M_2/M_1	Composition X_1	Composition X_2	λ_{exp} (mW ^{1} $m^{-1}K^{-1}$)	PD eqns (4) and (5)	CS
		0.6325	0 3675	33.81	−0 06	0
Ne–Ar	1.98	0.4724	0.5376	28.78	0 00	0
		0 2623	0.7377	23.36	0.17	0
		0.7762	0.2238	95.26	0.26	0
He-Ar	9.98	0.6547	0.3453	74.95	0.95	1
		0.3597	0.6403	41.04	−0 46	−0
		0.1895	0.8105	28.80	0 43	0

pages 268 and 266 of Millat *et al* (1996)]

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